

1,2,3-Trichloropropene
96-19-5 | DTXSID3047766

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.64

Global applicability domain: Inside

Local applicability domain index: 4.68e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1,2-Trichloroethane</div> <div>Measured: 1.89</div> <div>Predicted: 1.86</div>	<div>Image not found</div> <div>(Z)-1,2-Dichloroethylene</div> <div>Measured: 1.86</div> <div>Predicted: 1.82</div>	<div>Image not found</div> <div>(E)-1,2-Dichloroethylene</div> <div>Measured: 1.86</div> <div>Predicted: 1.82</div>
<div>Image not found</div> <div>Trichloroacetic acid</div> <div>Measured: 1.33</div> <div>Predicted: 1.41</div>	<div>Image not found</div> <div>Chloral</div> <div>Measured: 0.99</div> <div>Predicted: 1.18</div>	<div>Image not found</div> <div>1,4-Dichloro-2-butyne</div> <div>Measured: 2.01</div> <div>Predicted: 2.05</div>